



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:39 AM UTC

PDB ID : 2Y48 / pdb_00002y48
Title : Crystal structure of LSD1-CoREST in complex with a N-terminal SNAIL peptide
Authors : Baron, R.; Binda, C.; Tortorici, M.; McCammon, J.A.; Mattevi, A.
Deposited on : 2011-01-05
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

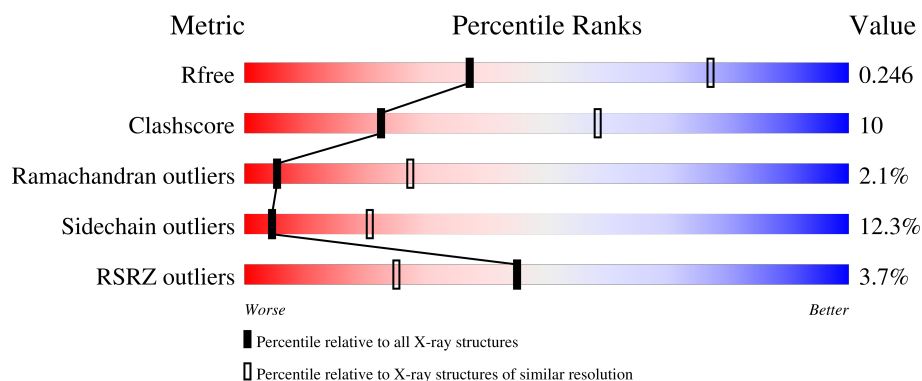
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	730	2% 63% 25% 9%
2	B	178	8% 46% 24% 25%
3	C	20	5% 30% 5% 10% 55%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6416 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called LYSINE-SPECIFIC DEMETHYLASE 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	665	Total	C	N	O	S	0	0	0
			5210	3319	905	966	20			

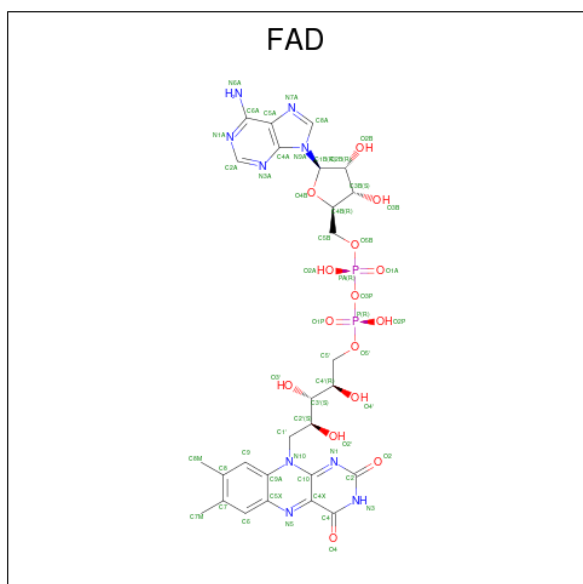
- Molecule 2 is a protein called REST COREPRESSOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

- Molecule 3 is a protein called ZINC FINGER PROTEIN SNAI1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			77	51	16	10			

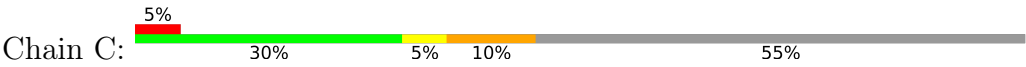
- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

GLU
ALA
PRO
VAL
LEU
ASP
VAL
ARG
TYR
ALA
SER
ALA
SER

● Molecule 3: ZINC FINGER PROTEIN SNAI1



P1	P2	P3	P4	P5	P6	P7	P8	P9	SER	ASP	PRO	ASN	ARG	LYS	PRO	ASN	TYR	SER	GLU

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.17Å 181.46Å 234.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.77 – 3.00 71.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (71.77-3.00) 99.5 (71.77-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.246 0.207 , 0.246	Depositor DCC
R_{free} test set	992 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6416	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.83	0/5323	1.05	13/7221 (0.2%)
2	B	0.63	0/1091	0.93	1/1471 (0.1%)
3	C	0.92	0/79	0.95	0/104
All	All	0.80	0/6493	1.03	14/8796 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	634	PRO	CA-C-N	9.30	129.38	119.90
1	A	634	PRO	C-N-CA	9.30	129.38	119.90
1	A	613	THR	N-CA-C	6.50	120.10	110.48
1	A	660	ASN	N-CA-C	6.28	119.76	109.85
1	A	440	GLU	N-CA-C	-6.02	104.84	111.82
1	A	770	GLY	N-CA-C	-5.94	107.54	115.32
1	A	273	LEU	CA-C-N	5.77	127.06	119.84
1	A	273	LEU	C-N-CA	5.77	127.06	119.84
2	B	327	ASN	N-CA-C	5.64	115.29	107.73
1	A	542	THR	CA-C-N	5.53	126.76	119.84
1	A	542	THR	C-N-CA	5.53	126.76	119.84
1	A	668	ARG	N-CA-C	5.45	117.37	108.55
1	A	492	LYS	N-CA-C	-5.26	105.19	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	834	TYR	N-CA-C	5.19	119.37	113.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	792	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5210	0	5244	121	0
2	B	1076	0	1091	24	0
3	C	77	0	89	3	0
4	A	53	0	31	5	0
All	All	6416	0	6455	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:SER:HB2	4:A:900:FAD:HM82	1.37	1.01
1:A:794:PRO:HD2	1:A:828:GLN:NE2	1.81	0.96
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.54	0.87
1:A:384:ARG:HB3	2:B:314:MET:HE1	1.56	0.85
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.91	0.83
1:A:270:ILE:O	1:A:272:PRO:HD3	1.77	0.83
1:A:494:TYR:CD1	1:A:494:TYR:O	2.36	0.78
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.48	0.76
1:A:453:GLU:HA	1:A:453:GLU:OE1	1.87	0.74
1:A:384:ARG:HB3	2:B:314:MET:CE	2.16	0.74
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:HA	4:A:900:FAD:N5	2.04	0.72
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.25	0.71
1:A:384:ARG:NH1	2:B:312:LYS:O	2.22	0.70
1:A:693:LEU:HD12	1:A:694:PHE:H	1.56	0.70
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.72	0.70
1:A:760:SER:CB	4:A:900:FAD:HM82	2.19	0.70
1:A:458:LEU:HB3	1:A:487:LEU:HD12	1.74	0.69
1:A:606:ASN:HD22	1:A:609:SER:H	1.40	0.69
1:A:801:GLU:HG2	1:A:809:ALA:H	1.58	0.68
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.75	0.66
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.29	0.66
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.36	0.65
1:A:537:GLU:HG2	1:A:544:LEU:HD21	1.77	0.65
1:A:656:PHE:CE2	1:A:759:GLY:HA3	2.32	0.64
1:A:331:ALA:HA	4:A:900:FAD:C4X	2.28	0.64
1:A:392:LEU:HD23	1:A:398:PHE:HD2	1.63	0.64
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.30	0.61
1:A:209:VAL:O	1:A:213:ILE:HG13	2.00	0.61
1:A:448:MET:HE2	2:B:363:LEU:HD13	1.84	0.59
1:A:537:GLU:HG2	1:A:544:LEU:CD2	2.33	0.58
1:A:666:PHE:O	1:A:701:PRO:HG2	2.04	0.58
1:A:601:GLU:HA	1:A:616:TYR:O	2.04	0.58
1:A:693:LEU:HD12	1:A:694:PHE:N	2.18	0.57
1:A:438:GLN:HG2	2:B:352:ILE:HG22	1.87	0.56
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.88	0.56
1:A:402:ASN:O	1:A:403:ASN:HB2	2.07	0.55
1:A:671:TRP:O	1:A:673:PRO:HD3	2.06	0.55
1:A:794:PRO:CD	1:A:828:GLN:NE2	2.64	0.54
1:A:468:VAL:O	1:A:472:ARG:NH1	2.41	0.54
1:A:808:PRO:O	1:A:810:THR:HG23	2.09	0.53
1:A:379:GLU:OE1	3:C:7:ARG:NH1	2.43	0.52
1:A:289:SER:HB3	1:A:814:ALA:HB1	1.91	0.52
1:A:435:VAL:HG12	2:B:349:ILE:HG13	1.91	0.52
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.93	0.51
1:A:662:VAL:HG13	1:A:748:VAL:HG22	1.92	0.51
1:A:548:SER:O	1:A:552:TRP:HB3	2.11	0.50
1:A:646:TRP:CZ3	1:A:647:LYS:HE2	2.46	0.50
1:A:801:GLU:HG2	1:A:809:ALA:N	2.25	0.50
1:A:501:GLN:O	1:A:505:GLU:HB2	2.12	0.50
1:A:182:ARG:NH1	1:A:341:PRO:HD3	2.28	0.49
1:A:650:ALA:O	1:A:654:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:VAL:HG12	2:B:324:VAL:O	2.12	0.49
2:B:324:VAL:HG13	2:B:331:ALA:HA	1.95	0.49
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.42	0.49
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.42	0.49
1:A:419:GLN:HE22	2:B:315:PHE:H	1.59	0.49
1:A:693:LEU:HD21	3:C:6:VAL:HG21	1.95	0.49
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.75	0.49
1:A:351:MET:HB3	1:A:567:VAL:HG13	1.95	0.48
1:A:473:ASP:OD1	1:A:473:ASP:C	2.57	0.48
1:A:715:MET:HE3	1:A:723:ILE:HG12	1.96	0.48
1:A:297:LEU:HB2	1:A:304:VAL:HG21	1.96	0.47
1:A:455:ILE:HD11	1:A:490:LEU:O	2.14	0.47
1:A:435:VAL:HG13	2:B:349:ILE:HG13	1.96	0.47
1:A:606:ASN:HD21	1:A:608:ARG:HB2	1.80	0.47
2:B:317:SER:O	2:B:321:VAL:HG23	2.12	0.47
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.96	0.47
1:A:489:ALA:O	1:A:492:LYS:HB3	2.15	0.47
1:A:533:PHE:O	1:A:537:GLU:HG3	2.15	0.47
2:B:417:VAL:O	2:B:421:PHE:HD1	1.98	0.47
1:A:366:ASN:OD1	1:A:367:GLY:N	2.48	0.47
1:A:448:MET:HG3	1:A:497:LEU:HD23	1.97	0.47
1:A:351:MET:HA	1:A:569:ASN:HD21	1.78	0.46
1:A:777:ALA:HB2	1:A:803:THR:HB	1.97	0.46
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.80	0.46
1:A:568:ARG:NH1	1:A:699:LYS:HG2	2.30	0.46
1:A:175:GLU:HG2	1:A:185:HIS:CG	2.51	0.45
1:A:273:LEU:HA	1:A:274:PRO:HD2	1.68	0.45
1:A:815:LEU:C	1:A:815:LEU:HD13	2.42	0.45
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.97	0.45
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.52	0.45
1:A:563:SER:O	1:A:565:LEU:HD12	2.16	0.45
1:A:566:THR:HG21	1:A:697:LEU:HD13	1.99	0.45
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.66	0.44
1:A:210:PHE:CE1	1:A:252:VAL:HG22	2.53	0.44
1:A:815:LEU:C	1:A:815:LEU:CD1	2.91	0.44
2:B:421:PHE:O	2:B:425:ARG:HB2	2.18	0.44
1:A:374:LYS:O	1:A:378:VAL:HG23	2.18	0.44
1:A:506:GLU:C	1:A:508:LEU:H	2.24	0.44
1:A:685:THR:O	1:A:688:ARG:HG2	2.18	0.44
1:A:317:VAL:HG12	1:A:317:VAL:O	2.17	0.44
1:A:520:TYR:CE2	1:A:521:LEU:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.33	0.43
1:A:541:ALA:O	1:A:657:GLY:HA3	2.19	0.43
1:A:331:ALA:HA	4:A:900:FAD:C5X	2.49	0.43
1:A:720:ASP:O	1:A:724:VAL:HG23	2.19	0.43
1:A:669:VAL:HG11	1:A:673:PRO:HG3	1.99	0.43
1:A:320:PHE:CD1	1:A:747:VAL:HG21	2.53	0.43
1:A:613:THR:HG22	1:A:614:PHE:N	2.33	0.43
1:A:801:GLU:CG	1:A:809:ALA:HA	2.49	0.43
2:B:418:LYS:O	2:B:421:PHE:HB2	2.19	0.43
1:A:292:ALA:HB2	1:A:815:LEU:HD22	2.01	0.42
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.18	0.42
1:A:780:ILE:HB	1:A:796:LEU:HB3	2.01	0.42
1:A:379:GLU:O	1:A:382:PHE:HB3	2.18	0.42
1:A:469:LYS:HE3	1:A:469:LYS:HA	2.01	0.42
1:A:243:ASN:OD1	1:A:243:ASN:C	2.61	0.42
1:A:521:LEU:HD22	1:A:525:ASP:HB3	2.01	0.42
1:A:763:TYR:CE1	1:A:765:ALA:HB2	2.54	0.42
1:A:341:PRO:HG2	1:A:812:HIS:HB2	2.00	0.42
1:A:493:GLU:C	1:A:495:ASP:N	2.77	0.42
1:A:364:GLU:HA	1:A:681:VAL:HB	2.01	0.42
1:A:422:HIS:HA	1:A:425:ASP:HB2	2.01	0.42
3:C:6:VAL:O	3:C:7:ARG:HB2	2.19	0.42
2:B:315:PHE:C	2:B:316:LEU:HG	2.45	0.42
2:B:428:PHE:O	2:B:429:ASN:C	2.63	0.42
1:A:354:ALA:HB2	1:A:568:ARG:HD2	2.01	0.42
1:A:594:ARG:HA	1:A:640:VAL:O	2.20	0.42
2:B:380:ASN:OD1	2:B:381:ALA:N	2.53	0.42
1:A:451:LEU:C	1:A:453:GLU:N	2.74	0.41
1:A:601:GLU:CD	1:A:617:LYS:HE2	2.44	0.41
1:A:374:LYS:O	1:A:375:ASP:C	2.63	0.41
1:A:656:PHE:CE2	1:A:759:GLY:CA	3.01	0.41
1:A:506:GLU:C	1:A:508:LEU:N	2.79	0.41
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.55	0.41
1:A:271:LYS:O	1:A:272:PRO:C	2.62	0.41
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.94	0.41
1:A:606:ASN:ND2	1:A:609:SER:H	2.14	0.41
2:B:329:THR:C	2:B:331:ALA:N	2.78	0.41
2:B:395:ILE:HG22	2:B:433:VAL:HG12	2.03	0.41
1:A:601:GLU:OE2	1:A:617:LYS:HE2	2.21	0.40
2:B:317:SER:O	2:B:318:GLN:C	2.64	0.40
1:A:248:LEU:O	1:A:249:VAL:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ASP:OD2	1:A:685:THR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	663/730 (91%)	594 (90%)	58 (9%)	11 (2%)	7	32
2	B	131/178 (74%)	111 (85%)	15 (12%)	5 (4%)	2	15
3	C	7/20 (35%)	6 (86%)	0	1 (14%)	0	1
All	All	801/928 (86%)	711 (89%)	73 (9%)	17 (2%)	5	27

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	VAL
1	A	737	SER
2	B	429	ASN
1	A	364	GLU
1	A	274	PRO
2	B	425	ARG
2	B	439	ALA
3	C	3	SER
1	A	425	ASP
1	A	510	GLU
1	A	793	ILE
2	B	401	ASP
1	A	271	LYS
1	A	322	LYS
1	A	573	CYS
2	B	373	PRO

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Mol	Chain	Res	Type
1	A	272	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	565/623 (91%)	508 (90%)	57 (10%)	7	29
2	B	117/156 (75%)	91 (78%)	26 (22%)	1	5
3	C	9/20 (45%)	7 (78%)	2 (22%)	1	5
All	All	691/799 (86%)	606 (88%)	85 (12%)	4	21

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	206	THR
1	A	226	LYS
1	A	237	GLN
1	A	238	LEU
1	A	247	VAL
1	A	281	VAL
1	A	351	MET
1	A	352	GLU
1	A	356	ILE
1	A	374	LYS
1	A	380	GLN
1	A	392	LEU
1	A	417	GLN
1	A	423	VAL
1	A	429	GLU
1	A	433	LYS
1	A	437	THR
1	A	438	GLN
1	A	449	VAL
1	A	456	LYS

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Mol	Chain	Res	Type
1	A	458	LEU
1	A	469	LYS
1	A	479	LEU
1	A	482	SER
1	A	487	LEU
1	A	492	LYS
1	A	508	LEU
1	A	514	ASN
1	A	523	SER
1	A	526	ARG
1	A	538	PHE
1	A	563	SER
1	A	591	ARG
1	A	598	SER
1	A	610	THR
1	A	612	GLN
1	A	621	VAL
1	A	624	THR
1	A	633	GLN
1	A	638	GLN
1	A	645	GLU
1	A	652	GLN
1	A	667	ASP
1	A	675	VAL
1	A	683	SER
1	A	684	THR
1	A	696	ASN
1	A	704	LEU
1	A	706	LEU
1	A	714	ILE
1	A	778	GLN
1	A	786	ILE
1	A	793	ILE
1	A	811	VAL
1	A	815	LEU
1	A	836	LEU
2	B	308	ARG
2	B	316	LEU
2	B	317	SER
2	B	332	THR
2	B	334	VAL
2	B	337	GLN

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Mol	Chain	Res	Type
2	B	339	ASP
2	B	343	VAL
2	B	344	SER
2	B	347	ARG
2	B	349	ILE
2	B	350	GLN
2	B	352	ILE
2	B	355	THR
2	B	359	LEU
2	B	360	LYS
2	B	361	GLU
2	B	376	ILE
2	B	379	CYS
2	B	385	THR
2	B	386	GLU
2	B	414	VAL
2	B	422	VAL
2	B	426	ARG
2	B	432	GLU
2	B	436	GLU
3	C	3	SER
3	C	6	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	358	GLN
1	A	417	GLN
1	A	419	GLN
1	A	484	HIS
1	A	551	HIS
1	A	606	ASN
1	A	717	ASN
1	A	742	GLN
1	A	778	GLN
1	A	828	GLN
2	B	337	GLN
2	B	348	GLN
2	B	350	GLN
2	B	411	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	FAD	A	900	-	58,58,58	1.12	4 (6%)	85,89,89	1.75	21 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	A	900	-	-	0/34/50/50	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	900	FAD	C4X-N5	3.45	1.38	1.30
4	A	900	FAD	C2A-N1A	2.81	1.38	1.33
4	A	900	FAD	C10-N1	2.77	1.38	1.33
4	A	900	FAD	C8A-N7A	2.49	1.36	1.31

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	FAD	N3A-C2A-N1A	-6.59	118.60	128.58
4	A	900	FAD	N9A-C8A-N7A	-3.95	108.34	113.94
4	A	900	FAD	C5A-C4A-N3A	-3.92	121.32	126.72
4	A	900	FAD	C2A-N3A-C4A	3.72	120.90	111.83
4	A	900	FAD	C4-N3-C2	-3.46	119.50	125.64
4	A	900	FAD	C5'-C4'-C3'	-3.06	106.44	112.22
4	A	900	FAD	C5A-N7A-C8A	3.03	108.21	103.45
4	A	900	FAD	O4-C4-C4X	-2.92	118.81	126.53
4	A	900	FAD	C5X-C9A-N10	2.83	120.52	117.97
4	A	900	FAD	N3A-C4A-N9A	2.76	131.86	127.17
4	A	900	FAD	C4A-N9A-C8A	2.75	108.62	105.74
4	A	900	FAD	C4X-C4-N3	2.53	119.69	113.25
4	A	900	FAD	O3'-C3'-C2'	2.51	114.62	108.93
4	A	900	FAD	C4-C4X-C10	2.33	120.92	116.93
4	A	900	FAD	C4A-C5A-N7A	-2.27	107.98	110.58
4	A	900	FAD	O4B-C1B-N9A	-2.26	103.75	108.09
4	A	900	FAD	O3B-C3B-C4B	-2.25	104.61	111.08
4	A	900	FAD	C4X-C10-N1	-2.24	119.10	124.59
4	A	900	FAD	C9A-C5X-N5	-2.22	120.10	122.45
4	A	900	FAD	C4'-C3'-C2'	-2.11	110.07	113.57
4	A	900	FAD	C2A-N1A-C6A	2.09	122.17	118.73

There are no chirality outliers.

There are no torsion outliers.

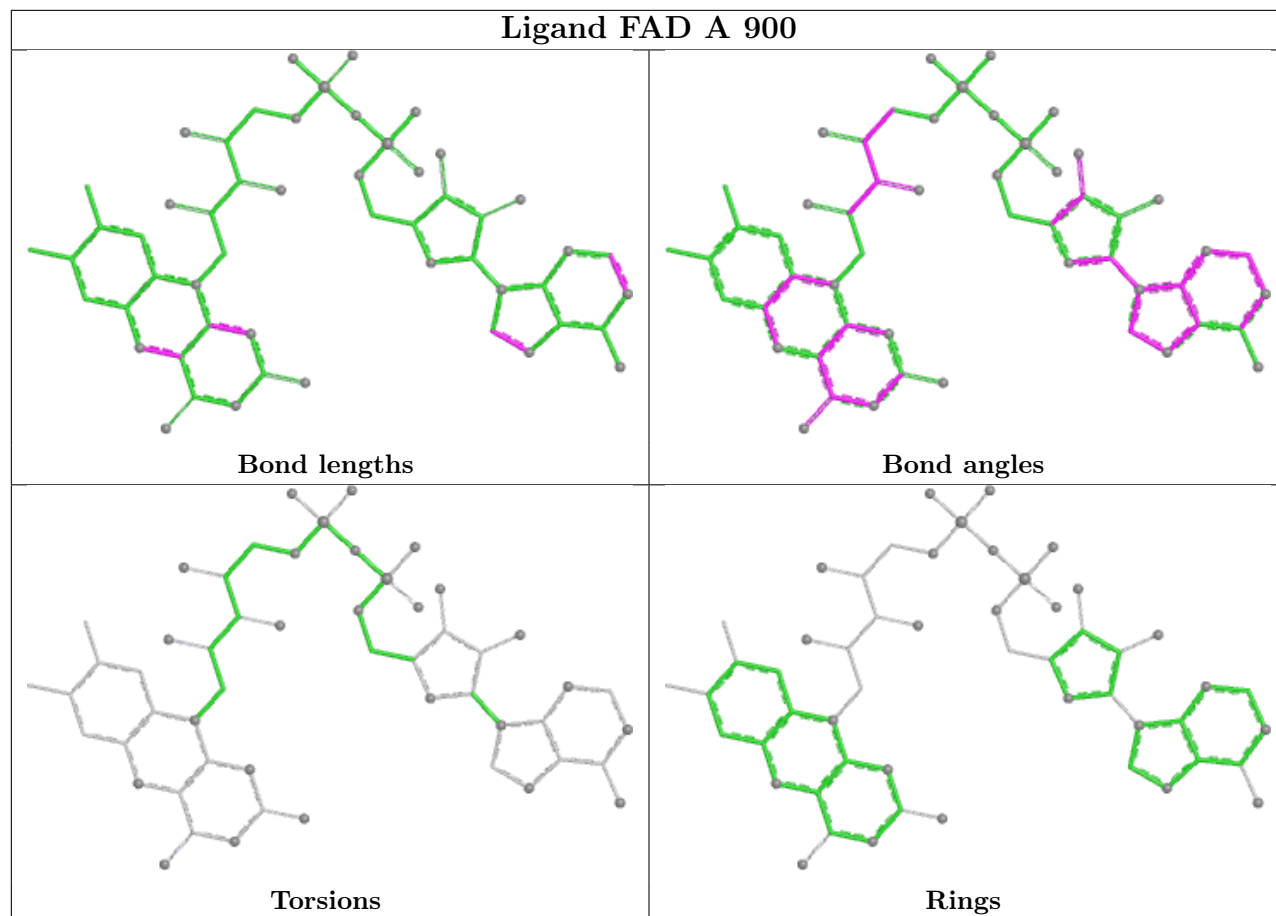
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	900	FAD	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	665/730 (91%)	-0.01	15 (2%) 61 38	41, 69, 100, 115	0
2	B	133/178 (74%)	0.79	14 (10%) 11 6	72, 104, 119, 127	0
3	C	9/20 (45%)	0.14	1 (11%) 10 6	63, 66, 91, 91	0
All	All	807/928 (86%)	0.12	30 (3%) 45 25	41, 76, 111, 127	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	6.3
1	A	275	THR	4.7
1	A	377	MET	4.6
1	A	373	GLU	4.1
2	B	312	LYS	4.0
2	B	440	GLU	3.5
2	B	376	ILE	3.3
2	B	337	GLN	3.3
2	B	431	ASP	3.1
2	B	374	GLU	3.1
1	A	511	LEU	2.9
1	A	833	MET	2.9
2	B	332	THR	2.6
2	B	379	CYS	2.5
2	B	340	MET	2.5
1	A	172	SER	2.5
1	A	507	LYS	2.4
2	B	386	GLU	2.4
1	A	239	GLU	2.3
1	A	440	GLU	2.2
1	A	376	GLU	2.2
1	A	205	GLN	2.1
1	A	506	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	8	LYS	2.1
2	B	308	ARG	2.1
2	B	399	GLY	2.1
2	B	375	VAL	2.0
1	A	403	ASN	2.0
1	A	739	ALA	2.0
2	B	320	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

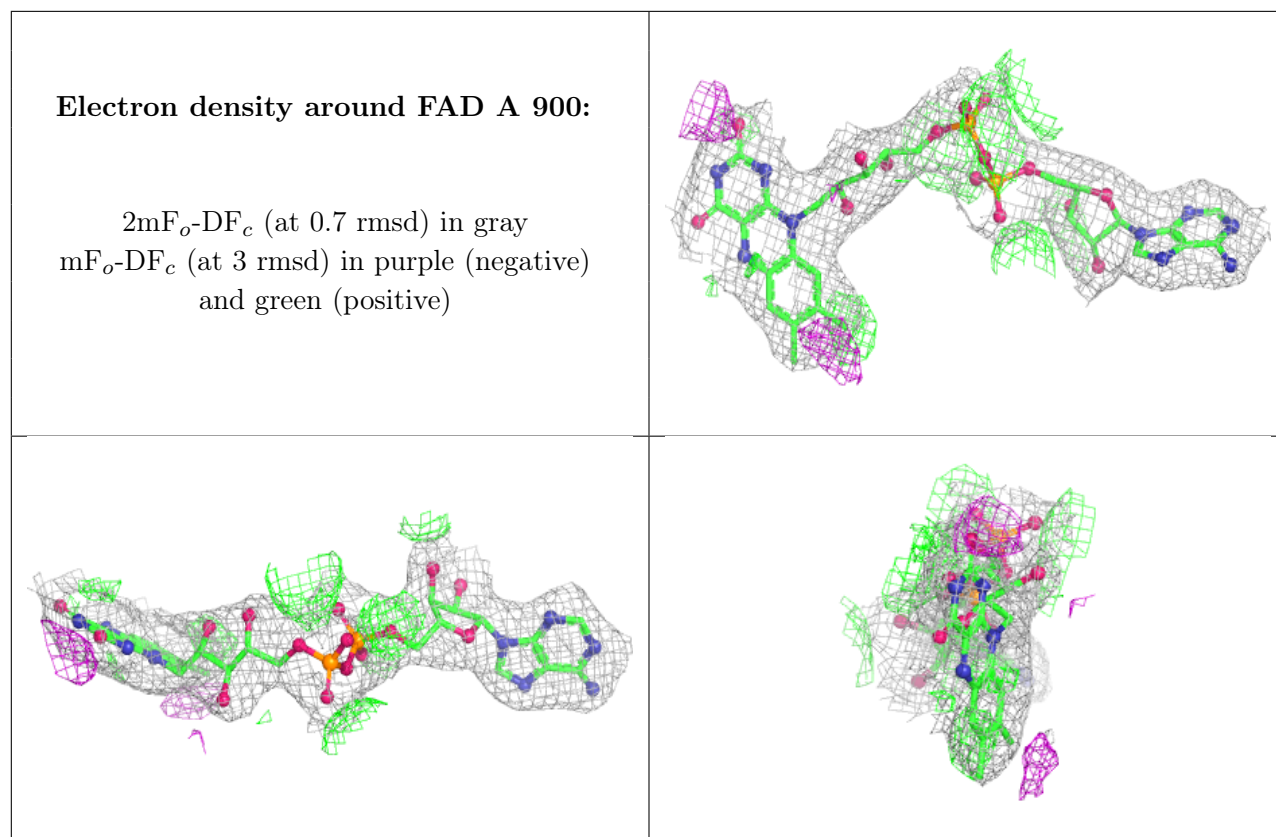
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FAD	A	900	53/53	0.97	0.07	38,42,59,60	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.